Winter 2-2005

Spectrometer Curve Smoothing Using Replicate Scans and Running Averages

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SPECTROMETER CURVE SMOOTHING USING REPLICATE SCANS AND RUNNING AVERAGES

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SUMMARY
The Boxcar Pixel Smoothing algorithm significantly reduced noise in spectral traces. However, averaging replicate scans did not significantly reduce noise in these studies.

INTRODUCTION
Two techniques are commonly used to reduce noise in spectral measurements: 1) averaging replicate scans and 2) the use of smoothing algorithms. We examined the advantages and disadvantages of curve smoothing by each of these techniques.

Spectrawiz, the software package available with Apogee-StellarNet spectrometers, allows users to reduce noise in spectra using two methods:

1) averaging up to 99 replicate scans
2) running average smoothing algorithm called Boxcar Pixel Smoothing.

There are five smoothing levels numbered from 0 to 4, which correspond to 1 to 33 pixels averaged. Pixels are specific locations on the sensor where the signal intensity is interpreted by the spectrometer. The relationship between nanometers and pixels is determined by the distance between each pixel. The width in nanometers between each pixel is not identical throughout the spectrum and varies slightly between individual spectrometers. The unit calibration coefficients provided with each spectrometer help establish the relationship between pixels and nanometers for individual spectrometers.

Setting	nm Smoothing Range	Total Pixels Averaged
0	0.4	1
1	2.1	5
2	3.7	9
3	7.0	17
4	13.6	33

MATERIALS AND METHODS
All spectral traces were measured with both an Apogee-StellarNet UV/VIS and a VIS/NIR spectrometer. An Apogee reflectance probe was used to collect spectra from the VIS/NIR spectrometer. Sunlight was used with the UV/VIS spectrometer because of the lack of UV light produced by the radiation source in the reflectance probe.

RESULTS

Measurements were taken on a white PTFE (polytetrafluoroethylene) disc used as a reference. Spectra representing 2, 3, 4, and 5 scans averaged were taken (Figure 1).

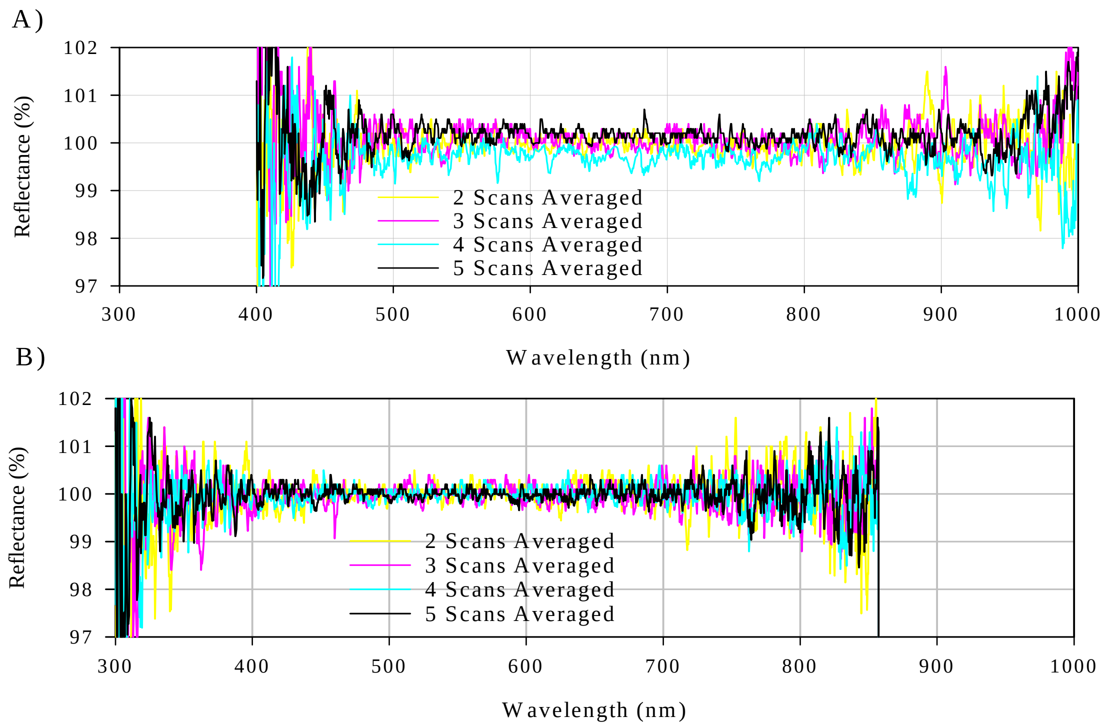


Figure 1. Spectra of white references representing different number of scans averaged from (A) VIS/NIR and (B) UV/VIS Apogee-StellarNet Spectrometers. No smoothing was used for these spectra.

White references were also smoothed in a spreadsheet using a running average (Figure 2).

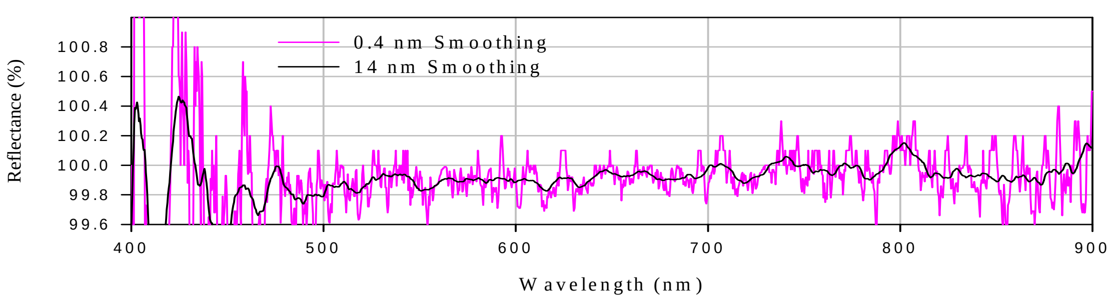


Figure 2. Spectra of white PTFE (polytetrafluoroethylene) used as a white reference. Spectra shown are an average of 5 scans and smoothed in a spreadsheet.

MEASUREMENTS ON ROSCOLUX FILTERS

Measurements were taken on each of five different colors that had reflectance spectra similar to plant leaves (primary green #91, moss green #89, pea green #86, light green #88 and pale yellow green #87) of plastic Roscolux filters (Figure 3; http://www.rosco.com/us/filters/filters-roscolux.asp). Roscolux plastic filters were used as a leaf model because of their uniformity and reproducibility.

Figure 3. Roscolux Colored Filters.

Measurements were taken on each filter color with each of the five smoothing levels (Figure 4). The raw data (no smoothing) of pea green (#86) was also smoothed in a spreadsheet using a running average similar to the Spectrawiz software (Figure 5). This was done to provide a more direct comparison between smoothed and unsmoothed spectra. The pea green filter was studied more extensively because it most closely resembled the curve of a leaf.

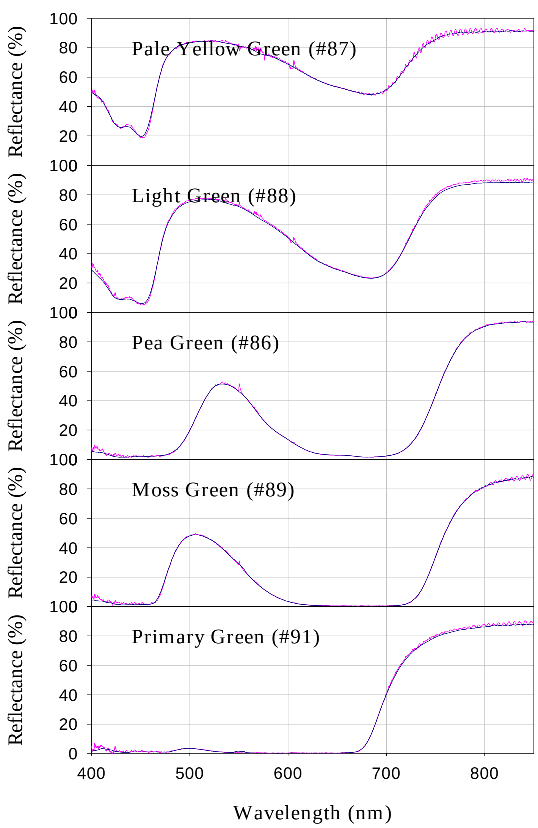


Figure 4. The spectra of Roscolux colored filters with no spectral smoothing and smoothed by a running average of 33 (about 14 nm) pixels. Each spectrum shown is an average of 5 spectra and was measured with a UV/VIS spectrometer.

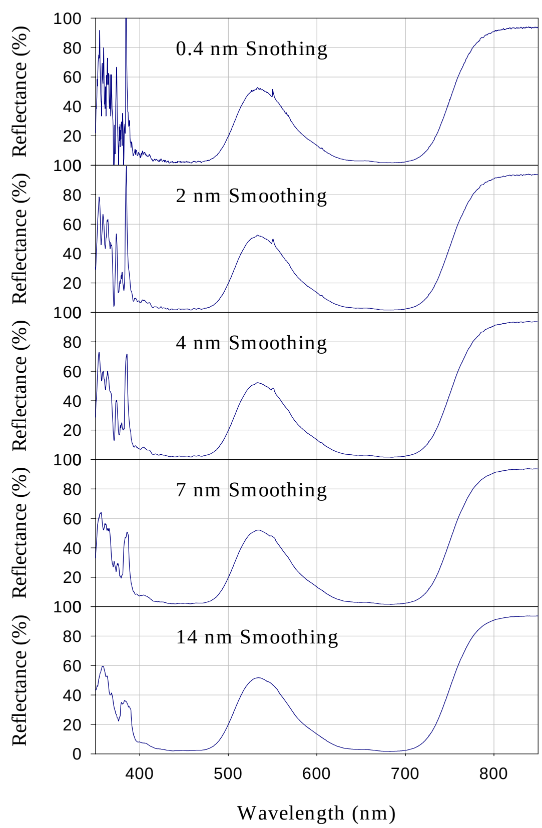


Figure 5. The spectra of Roscolux pea green #86 with no spectral smoothing and four levels of smoothing done in a spreadsheet. Each spectrum was measured with a UV/VIS spectrometer.

Replicate Scan Averaging

Replicate scan averaging of spectra reduced noise from 400 nm to 450 nm and between 800 nm and 1000 nm using the VIS/NIR spectrometer (Figure 6).

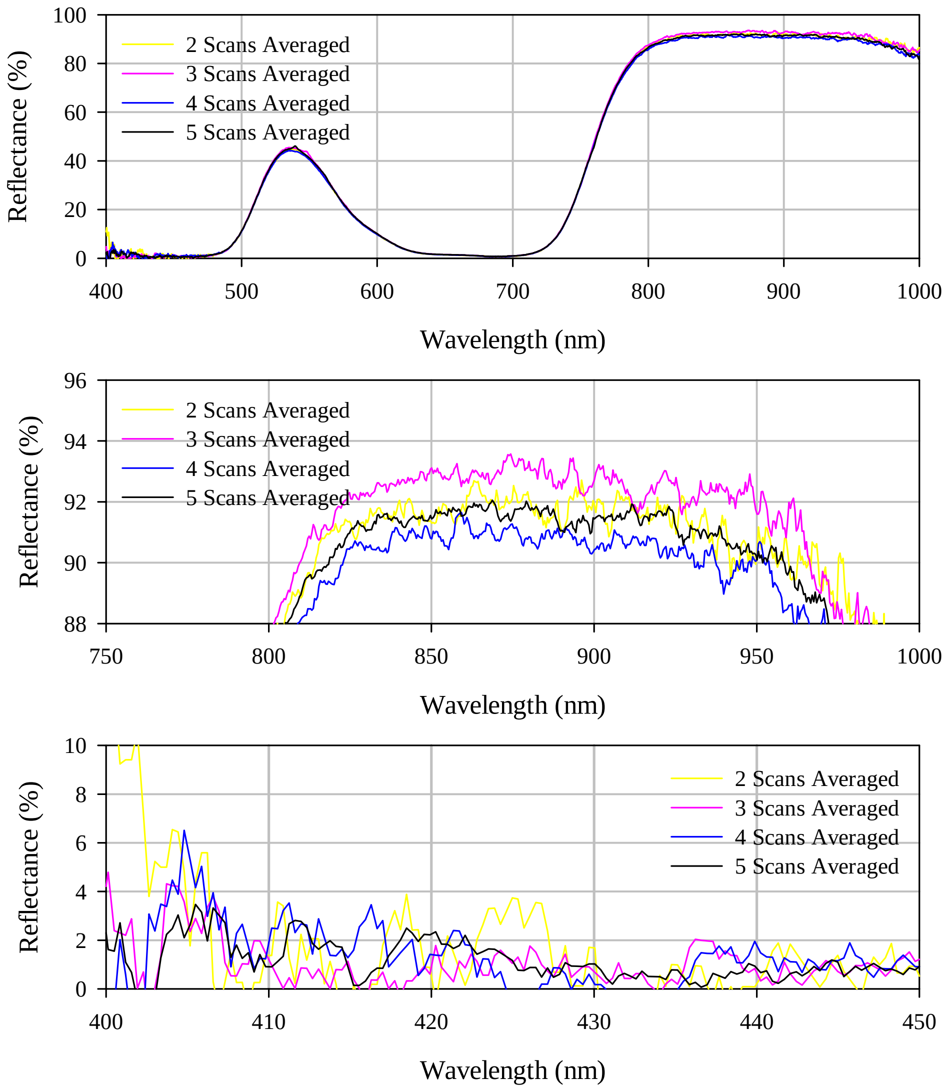


Figure 6. Spectra of Roscolux pea green (#86) colored filter measured with Apogee-StellarNet VIS/NIR Spectrometer. Averaging more than one scan only slightly reduces noise.

Boxcar Pixel Smoothing

Spectral smoothing reduced the noise below 450 nm in spectra of both filters (Figure 7). Smoothing also improved the infrared portion of the filter spectra (Figure 8).

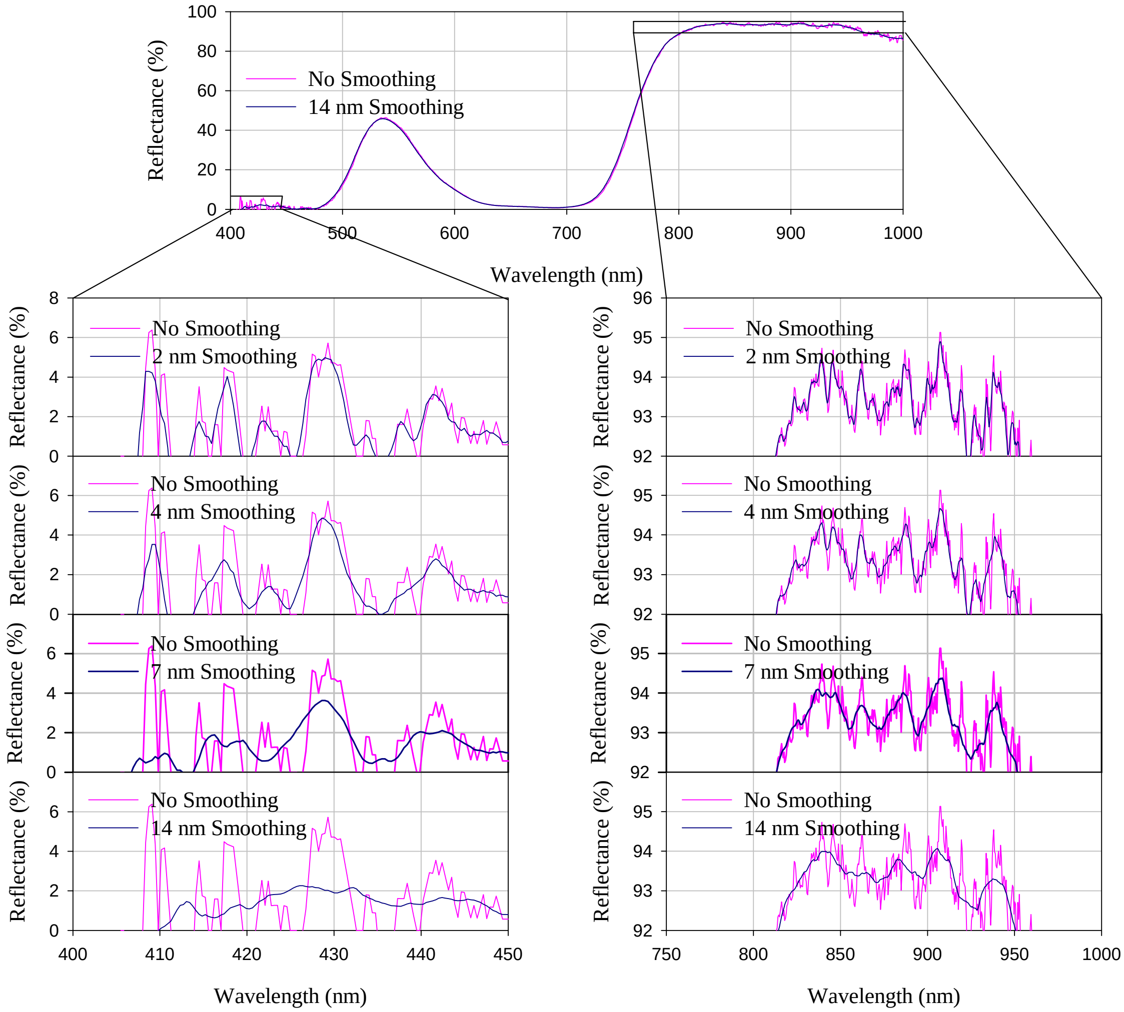


Figure 7. The spectra of Roscolux pea green #86A acetate between 400 nm and 450 nm with no spectral smoothing and 4 levels of smoothing done in a spreadsheet. Spectra measured with the VIS/NIR spectrometer.

Figure 8. The spectra of Roscolux pea green #86A acetate from 750 nm to 1000 nm with no spectral smoothing and 4 levels of smoothing done in a spreadsheet. Measured with the VIS/NIR spectrometer.

Spectral smoothing had an effect on the sharp curve near 700 nm (Figure 9). Smoothing in this area is significant because sharp corners are rounded by smoothing. The curve near 700 nm, often called the “red edge”, can be used as an indicator of plant health (Datt, 1999). Running-averages cause sharp corners to become rounded. This occurred to some extent with this smoothing algorithm.

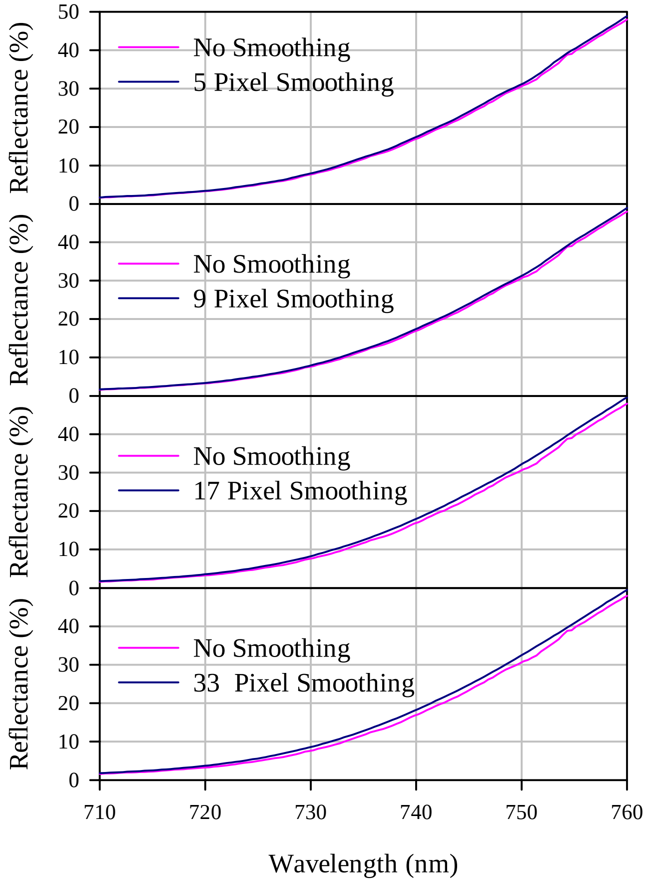
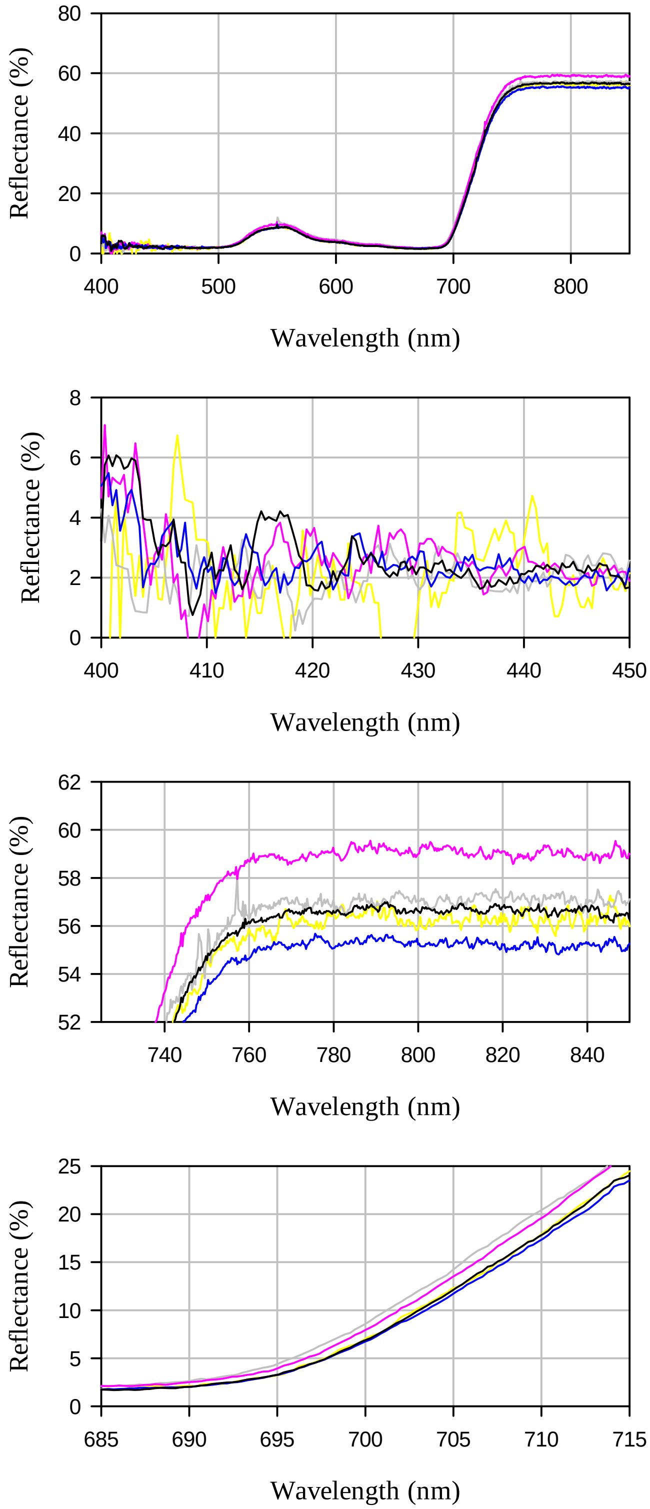


Figure 9. The spectra of Roscolux pea green #86A between 710 nm and 760 nm with no smoothing and four levels of spectral smoothing done in a spreadsheet for direct comparison.

Measurements on Leaves

Measurements were also taken on leaves of a ficus benjamina tree. Results on leaves were similar to those on plastic filters. Averaging scans of leaf spectra reduced noise from 400 nm to 450 nm, from 750 nm to 850 nm, but did affect the red edge curve (Figure 10). Offsets in the spectra are not caused by the effects of averaging. They are caused by the effects of experimental error in measuring multiple spectra.



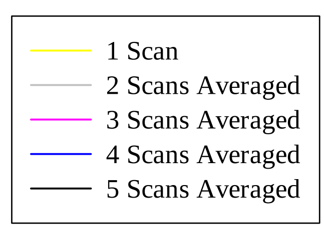


Figure 10. Spectra of ficus benjamina averaged in Spectrawiz. Measurements of leaves show results similar to measurements of Roscolux plastic filters.

Smoothing on leaves also showed results similar to smoothing on plastic filters (Figure 11). Noise between 400 nm and 450 nm was reduced. Noise in the near infrared portion of the spectrum was reduced from 750 nm to 850 nm with the UV/VIS spectrometer and from 750 nm to 1000 nm in the VIS/NIR spectrometer. The red edge curve (near 700 nm) was affected similarly to the effect in the plastic filters (Figure 12).

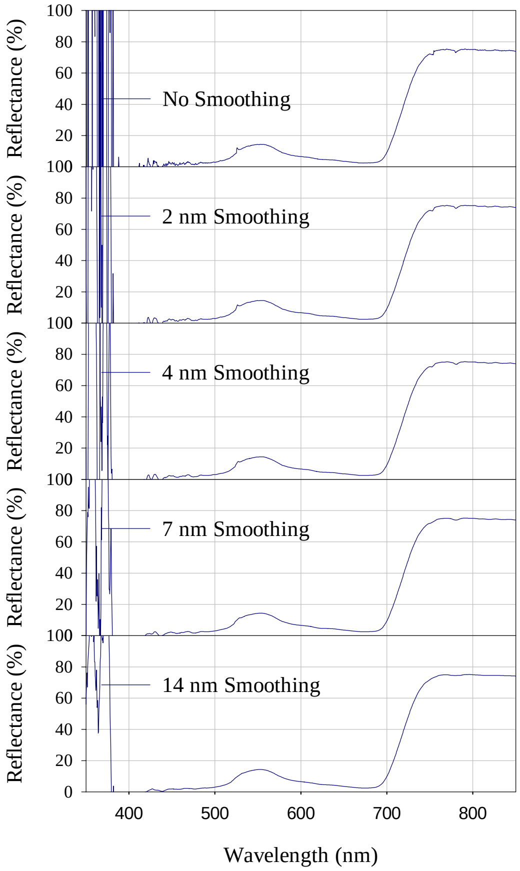


Figure 11. Spectra of *ficus benjamina* smoothed in a spreadsheet for direct comparison at four different smoothing levels. Spectra measured with VIS/NIR spectrometer.

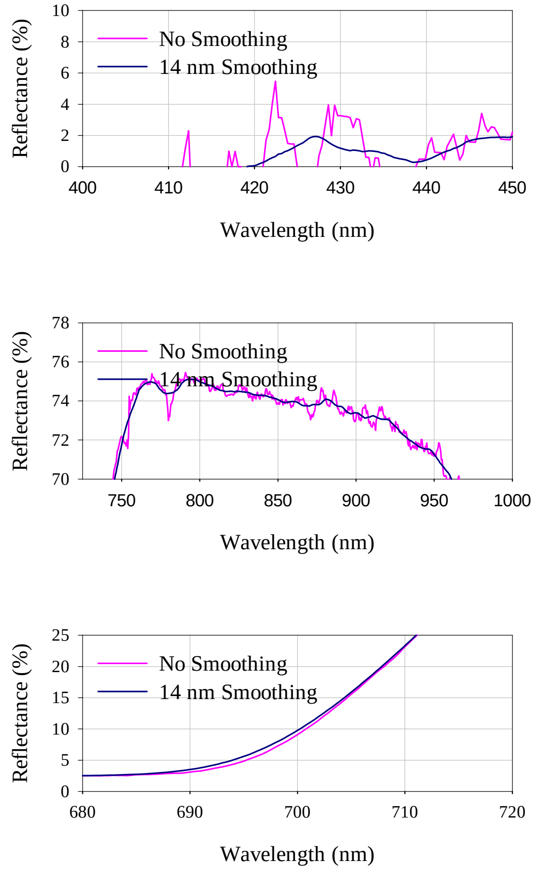


Figure 12. Spectra of *ficus benjamina* smoothed in a spreadsheet and an unsmoothed spectrum measured with VIS/NIR spectrometer. The effects of smoothing on leaves are similar to those on plastic filters.

Effects on Vegetative Indices

Slight changes in vegetative indices occurred with increasing smoothing. Indices with wavelengths closer to the UV were more affected (Figure 13).

Index	0.4 nm	2 nm	4 nm	7 nm	14 nm	Mean	St. Dev.	CV
NCPI(R680-R430)/(R680+R430)	-0.136	-0.149	-0.116	0.018	0.365	-0.003	0.194	-5856.5
PRI(R550-R530)/(R550+R530)	0.125	0.123	0.120	0.114	0.113	0.119	0.005	3.88
MCARI(R700-R670)-0.2(R700-R550)*(R700/R670)	10.4	10.5	10.5	10.6	10.7	10.5	0.079	0.747
NDVI(R850-R700)/(R850+R700)	0.782	0.782	0.781	0.779	0.768	0.778	0.005	0.664
940/650	20.3	20.3	20.3	20.1	20.0	20.2	0.133	0.657
RVIg/r	0.172	0.172	0.171	0.171	0.173	0.172	0.001	0.500
RVIr/g	5.81	5.83	5.85	5.85	5.77	5.82	0.029	0.499
DattR675/(R550*R708)	0.009	0.009	0.008	0.008	0.008	0.008	0.000	0.489
RVIred	30.0	30.1	30.3	30.3	30.1	30.2	0.137	0.454
RVIgreen	5.16	5.16	5.18	5.19	5.22	5.18	0.022	0.433
Chl NDI	0.510	0.510	0.509	0.507	0.504	0.508	0.002	0.391
DVIgreen	59.5	59.6	59.6	59.7	59.9	59.7	0.126	0.212
NDVIgreen	0.675	0.676	0.676	0.677	0.679	0.676	0.001	0.173
NGR	1.39	1.39	1.38	1.38	1.38	1.38	0.002	0.164
DVIred	71.4	71.4	71.5	71.6	71.6	71.5	0.084	0.117
Datt(IR-710)/(IR-R675)	0.706	0.706	0.707	0.706	0.705	0.706	0.001	0.101
DVIg/r	0.834	0.834	0.834	0.835	0.836	0.835	0.001	0.099
DVIr/g	1.20	1.20	1.20	1.20	1.20	1.20	0.001	0.098
NDVIred	0.935	0.936	0.936	0.936	0.936	0.936	0.000	0.030

Figure 13. Spectral indices are affected by smoothing. This data corresponds to spectra shown in Figures 11 and 12.

Correlations between Minolta SPAD-502 chlorophyll meter, which shows a high correlation to chlorophyll levels (Richardson et. al. 2002; Monje and Bugbee 1992), and vegetative indices at each smoothing level were calculated. Of the 20 indices tested, 13 showed a slight increase in correlation to the SPAD value after smoothing (Figure 14).

Index	0.4 nm	2 nm	4 nm	7 nm	14 nm
NDVI(850-700)/(850+700)	0.9682	0.9683	0.9686	0.9687	0.969
NDVIgreen	0.9668	0.9669	0.9668	0.9668	0.967

Datt(IR-710)/(IR-red)	0.9625	0.9632	0.9634	0.9636	0.9638
Chl NDI	0.9657	0.9659	0.9652	0.9644	0.9635
D730	0.7784	0.9132	0.956	0.947	0.9594
DVIg/r	0.9564	0.9562	0.9562	0.9565	0.9572
NGR	0.9084	0.9086	0.9087	0.9014	0.9139
DVIgreen	0.9068	0.9069	0.9052	0.9035	0.9028
DVIr/g	0.8952	0.8957	0.8958	0.8977	0.9014
RVIgreen	0.8716	0.8716	0.8739	0.8752	0.8747
940/650	0.5486	0.5525	0.5567	0.557	0.5584
Dattred/(green*R708)	0.5567	0.5545	0.5547	0.5547	0.5511
RVIr/g	0.3853	0.3842	0.3834	0.3838	0.3739
DVIred	0.3508	0.3509	0.3457	0.3412	0.3446
NDVIred	0.323	0.3258	0.3239	0.3215	0.3349
RVIg/r	0.2678	0.2666	0.2644	0.2652	0.2598
RVIred	0.1597	0.1619	0.1588	0.157	0.1744
MCARI(700-670)-0.2(700-550)*(700/670)	0.1263	0.1194	0.1234	0.1342	0.1657
PRI(550-530)/(550+530)	0.1103	0.1162	0.1096	0.0934	0.078
NCPI(680-430)/(680+430)	0.023	0.0184	0.0005	0.11158	0.0683

Figure 14. Correlation of vegetative indices and Minolta SPAD-502 values. Indices in the gray boxes showed a decrease in correlation.

CONCLUSIONS

The Boxcar Pixel Smoothing algorithm significantly reduced noise in spectral traces. However, averaging replicate scans did not significantly reduce noise.

Boxcar Pixel smoothing primarily reduced noise at the ends of the spectrum. However, the red edge curve near 700 nm becomes slightly more rounded.

Increasing the number of scans that were averaged from one to two improved smoothing. The value of averaging scans depends on how much movement occurs between scans. If movement occurs between scans the response is changed. Therefore, at long integration times in low light it may be beneficial to average fewer scans. Vegetative indices were slightly affected by smoothing. The indices most affected by smoothing were those that use wavelengths close to the UV portion of the spectrum. Correlations of vegetative indices with the Minolta SPAD-502 chlorophyll meter improved in 13 of the 20 indices tested.

LITERATURE CITED

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